WHAT IS CLAIMED IS:

1. A computer program product on a computer-readable medium for designing a set of experiments, the program comprising instructions operable to cause a programmable processor to:

define a set of experimental parameters, one or more sampling patterns defining a sampling for each parameter of the set of experimental parameters, and one or more constraints limiting the set of experiments to a particular volume or volumes of a hyperspace defined by the set of experimental parameters, at least a plurality of the set of parameters being grouped according to a parameter type such that the grouped parameters are constrained to perform a common role in the set of experiments;

generate a first estimate of the practicability of a set of experiments defined by the parameters, the sampling patterns and the constraints, the first estimate including a count of the set of experiments defined by the set of experimental parameters, the sets of values and the constraints, and provide the first estimate to a user;

receive an input in response to the first estimate;

in response to an input modifying at least one of the set of parameters, the sampling patterns or the constraints, generate a second estimate of the practicability of the set of experiments and provide the second estimate to the user; and

in response to an input approving of the estimate, generate an experiment design defined by the parameters, the sampling patterns and the constraints, the experiment design including a final set of experiments.

2. The computer program product of claim 1, wherein:

the experiment design includes data representing a plurality of sets of coordinates in the hyperspace defined by the set of experimental parameters, each of the sets of coordinates defining an experiment in the final set of experiments, such that the experiment design is capable of being implemented to cause a computer-controlled combinatorial synthesis process to perform the final set of experiments.

3. The computer program product of claim 2, wherein:

the sampling patterns include at least a first sampling pattern defined for a first parameter of the set of experimental parameters and a second sampling pattern defined for a second parameter of the set of experimental parameters, wherein the first sampling pattern is different from the second sampling pattern.

4. The computer program product of claim 3, wherein:

at least one of the first and second sampling patterns includes a gradient of parameter values defined by a minimum parameter value, a maximum parameter value and a step size.

5. The computer program product of claim 4, wherein:

the first and second sampling patterns are defined by first and second gradients.

6. The computer program product of claim 2, wherein:

the set of experimental parameters includes a plurality of component materials to be used in the set of experiments.

7. The computer program product of claim 6, wherein:

the set of experimental parameters includes at least one process condition to be varied in the set of experiments.

8. The computer program product of claim 6, wherein:

the constraints include a mixture constraint limiting the fractional contribution of at least a plurality of the component materials to a total composition in one or more of the experiments in the set of experiments.

9. The computer program product of claim 8, wherein:

the mixture constraint specifies a minimum number of component materials to be included in one or more of the experiments in the set of experiments.

10. The computer program product of claim 9, wherein:

the mixture constraint specifies a maximum number of component materials to be included in one or more of the experiments in the set of experiments.

11. The computer program product of claim 6, wherein:

the constraints include a type constraint limiting the total number of parameters of a specified type to be included in one or more of the experiments in the set of experiments.

12. The computer program product of claim 6, wherein:

the constraints include a sum constraint limiting the sum of a contribution of parameters of a specified type to one or more of the experiments in the set of experiments.

13. The computer program of claim 6, wherein:

the constraints include a balance constraint limiting the contribution of at least one parameter to a plurality of experiments of the set of experiments based on the contribution of one or more other parameters to one or more of the experiments in the set of experiments.

14. The computer program product of claim 6, wherein:

the constraints include a list constraint identifying a list of one or more starting compositions to be used to generate the set of experiments.

15. The computer program product of claim 14, wherein:

each of the starting compositions is represented as a point in the hyperspace defined by the set of experimental parameters; and

the list constraint specifies a distance criterion specifying an acceptable distance in the hyperspace from the points corresponding to the starting compositions.

16. The computer program product of claim 14, wherein:

the one or more starting compositions are derived from results of a previous experiment.

17. The computer program product of claim 6, wherein:

the constraints include a synthesis constraint specifying an order in which a plurality of component materials are to be added in a synthesis to be performed in one or more of the experiments in the set of experiments.

18. The computer program product of claim 17, wherein:

the synthesis constraint specifies that the order in which component materials are to be added is to vary between a plurality of experiments in the set of experiments.

19. The computer program product of claim 6, wherein:

the constraints include a process constraint specifying an order in which a plurality of process steps are to be performed in one or more of the experiments in the set of experiments.

20. The computer program product of claim 19, wherein:

the process constraint specifies that the order in which process steps are to be performed is to vary between a plurality of experiments in the set of experiments.

21. The computer program product of claim 2, wherein:

the constraints include a project constraint specifying the order in which individual experiments in the set of experiments are to be performed.

22. The computer program product of claim 21, wherein:

the project constraint includes a priority value assigned to one or more of the set of experiment parameters, the priority value representing a relative priority attached to the corresponding parameter.

23. The computer program product of claim 6, wherein:

the constraints include one or more chemistry-specific constraints selected from the group including balance constraints, electron-counting constraints, atomic size constraints, ionic size constraints, atomic packing constraints, ionic packing constraints, heat of formation constraints, or entropy constraints.

24. The computer program product of claim 2, wherein:

at least one of the constraints includes one or more tolerance values representing an amount by which the corresponding constraint can be relaxed during generation of the experiment design.

25. The computer program product of claim 2, wherein the instructions operable to generate the experiment design include instructions operable to cause a programmable processor to:

identify a plurality of points in the hyperspace defined by the set of experimental parameters corresponding to candidate materials by counting through parameter space points defined by the sampling pattern and applying the experimental constraints to the parameter space points.

26. The computer program product of claim 2, wherein:

the set of experimental parameters includes at least four experimental parameters.

27. The computer program product of claim 2, wherein:

the set of experimental parameters includes at least six experimental parameters.

28. The computer program product of claim 2, wherein:

the set of experimental parameters includes at least ten experimental parameters.

29. The computer program product of claim 2, wherein:

the set of experimental parameters includes at least fifty experimental parameters.

30. The computer program product of claim 2, wherein:

the final set of experiments includes at least 48 experiments.

31. The computer program product of claim 2, wherein:

the final set of experiments includes at least 96 experiments.

32. The computer program product of claim 2, wherein:
the final set of experiments includes at least 1,000 experiments.

33. The computer program product of claim 2, wherein:
the final set of experiments includes at least 10,000 experiments.

34. The computer program product of claim 2, wherein:
the final set of experiments includes at least 50,000 experiments.

35. The computer program product of claim 2, wherein:
the final set of experiments includes at least 100,000 experiments.

36. The computer program product of claim 6, wherein:
each of the component materials has an associated set of material properties describing the component material; and
the instructions operable to cause a programmable processor to define the set of experimental parameters include instructions operable to cause a programmable processor to receive for each of the component materials a set of values for one or more of the material properties associated with the component material.

37. The computer program product of claim 36, wherein:
at least one of the material properties is selected from the group consisting of molecular weight, equivalents, density and concentration.

38. The computer program product of claim 36, wherein:
at least one of the material properties is a type describing a class of chemicals to be used in generating the experiment design.

39. A computer-implemented method for designing a set of experiments, comprising:
defining a set of experimental parameters, one or more sampling pattern defining a sampling for each parameter of the set of experimental parameters, and one or more

constraints limiting the set of experiments to a particular volume or volumes of a hyperspace defined by the set of experimental parameters, at least a plurality of the set of parameters being grouped according to a parameter type such that the grouped parameters are constrained to perform a common role in the set of experiments;

generating a first estimate of the practicability of a set of experiments defined by the parameters, the sampling patterns and the constraints, the first estimate including a count of the set of experiments defined by the set of experimental parameters, the sets of values and the constraints, and providing the first estimate to a user;

receiving an input in response to the first estimate;

in response to an input modifying at least one of the set of parameters, the sampling patterns or the constraints, generating a second estimate of the practicability of the set of experiments and providing the second estimate to the user; and

in response to an input approving of the estimate, generating an experiment design defined by the parameters, the sampling patterns and the constraints, the experiment design including a final set of experiments.

40. The method of claim 39, wherein:

the experiment design includes data representing a plurality of sets of coordinates in the hyperspace defined by the set of experimental parameters, each of the sets of coordinates defining an experiment in the final set of experiments, the method further comprising:

using the experiment design to synthesize one or more combinatorial libraries including a plurality of compositions defined by the coordinates of the experiment design.

41. The method of claim 40, wherein:

the sampling patterns include at least a first sampling pattern defined for a first parameter of the set of experimental parameters and a second sampling pattern defined for a second parameter of the set of experimental parameters, wherein the first sampling pattern is different from the second sampling pattern.

42. The method of claim 40, wherein:

the set of experimental parameters includes a plurality of component materials to be used in the set of experiments.

43. The method of claim 42, wherein:

the set of experimental parameters includes at least one process condition to be varied in the set of experiments.

44. The method of claim 42, wherein:

the constraints include a mixture constraint limiting the fractional contribution of at least a plurality of the component materials to a total composition in one or more of the experiments in the set of experiments.

45. The method of claim 42, wherein:

the constraints include a type constraint limiting the total number of parameters of a specified type to be included in one or more of the experiments in the set of experiments.

46. The method of claim 42, wherein:

the constraints include a sum constraint limiting the sum of a contribution of parameters of a specified type to one or more of the experiments in the set of experiments.

47. The method of claim 42, wherein:

the constraints include a balance constraint limiting the contribution of at least one parameter to a plurality of experiments of the set of experiments based on the contribution of one or more other parameters to one or more of the experiments in the set of experiments.

48. The method of claim 42, wherein:

the constraints include a list constraint identifying a list of one or more starting compositions to be used to generate the set of experiments.

49. The method of claim 42, wherein:

the constraints include a synthesis constraint specifying an order in which a plurality of component materials are to be added in a synthesis to be performed in one or more of the experiments in the set of experiments.

50. The method of claim 49, wherein:

the synthesis constraint specifies that the order in which component materials are to be added is to vary between a plurality of experiments in the set of experiments.

51. The method of claim 42, wherein:

the constraints include a process constraint specifying an order in which a plurality of process steps are to be performed in one or more of the experiments in the set of experiments.

52. The method of claim 51, wherein:

the process constraint specifies that the order in which process steps are to be performed is to vary between a plurality of experiments in the set of experiments.

53. The method of claim 40, wherein:

the constraints include a project constraint specifying the order in which individual experiments in the set of experiments are to be performed.

54. The method of claim 40, wherein:

at least one of the constraints includes one or more tolerance values representing an amount by which the corresponding constraint can be relaxed during generation of the experiment design.

55. The method of claim 40, wherein:

generating the experiment design includes identifying a plurality of points in the hyperspace defined by the set of experimental parameters corresponding to candidate materials by counting through parameter space points defined by the sampling pattern and applying the experimental constraints to the parameter space points.

56 The method of claim 40, wherein:
the set of experimental parameters includes at least four experimental parameters.

57 The method of claim 40, wherein:
the set of experimental parameters includes at least six experimental parameters.

58. The method of claim 40, wherein:
the set of experimental parameters includes at least ten experimental parameters.

59. The method of claim 40, wherein:
the set of experimental parameters includes at least fifty experimental parameters.

60. The method of claim 40, wherein:
the final set of experiments includes at least 48 experiments.

61. The method of claim 40, wherein:
the final set of experiments includes at least 96 experiments.

62. The method of claim 40, wherein:
the final set of experiments includes at least 1,000 experiments.

63. The method of claim 40, wherein:
the final set of experiments includes at least 10,000 experiments.

64. The method of claim 40, wherein:
the final set of experiments includes at least 50,000 experiments.

65. The method of claim 40, wherein:
the final set of experiments includes at least 100,000 experiments.

66. The method of claim 42, wherein:

each of the component materials has an associated set of material properties describing the component material; and

defining the set of experimental parameters includes receiving for each of the component materials a set of values for one or more of the material properties associated with the component material.

67. The method of claim 66, wherein:

at least one of the material properties is selected from the group consisting of molecular weight, equivalents, density and concentration.

68. The method of claim 66, wherein:

at least one of the material properties is a type describing a class of chemicals to be used in generating the experiment design.

69. A computer-implemented method for designing a set of experiments, comprising:

defining a set of experimental parameters, at least a plurality of the set of parameters being grouped according to a parameter type such that the grouped parameters are constrained to perform a common role in the set of experiments, and identifying the parameters to an experiment design system;

selecting one or more sampling patterns defining a sampling for each of the parameters and providing the sampling patterns as input to the system;

defining one or more constraints limiting experiments in the set of experiments to a particular volume or volumes of a hyperspace defined by the set of experimental parameters and providing the definition of the constraints to the system;

receiving from the system an estimate of the practicability of the set of experiments defined by the parameters, the sampling patterns and the constraints, the first estimate including a count of the set of experiments defined by the set of experimental parameters, the sets of values and the constraints;

if the estimate indicates that the set of experiments is not practicable, modifying at least one of the set of parameters, the sampling patterns or the constraints, and receiving a second estimate of the practicability of the set of experiments; and

if the estimate indicates that the set of experiments is practicable, approving of the estimate, and an experiment design defined by the parameters, the sampling patterns and the constraints, the experiment design including a final set of experiments.

70. The method of claim 69, wherein:

the experiment design includes data representing a plurality of sets of coordinates in the hyperspace defined by the set of experimental parameters, each of the sets of coordinates defining an experiment in the final set of experiments, the method further comprising:

using the experiment design to synthesize one or more combinatorial libraries including a plurality of compositions defined by the coordinates of the experiment design.

71. The method of claim 70, wherein:

the sampling patterns include at least a first sampling pattern defined for a first parameter of the set of experimental parameters and a second sampling pattern defined for a second parameter of the set of experimental parameters, wherein the first sampling pattern is different from the second sampling pattern.

72. The method of claim 70, wherein:

the set of experimental parameters includes a plurality of component materials to be used in the set of experiments.

73. The method of claim 72, wherein:

the set of experimental parameters includes at least one process condition to be varied in the set of experiments.

74. The method of claim 72, wherein:

the constraints include a mixture constraint limiting the fractional contribution of at least a plurality of the component materials to a total composition in one or more of the experiments in the set of experiments.

75. The method of claim 72, wherein:

the constraints include a type constraint limiting the total number of parameters of a specified type to be included in one or more of the experiments in of the set of experiments.

76. The method of claim 72, wherein:

the constraints include a sum constraint limiting the sum of a contribution of parameters of a specified type to one or more of the experiments in the set of experiments.

77. The method of claim 72, wherein:

the constraints include a balance constraint limiting the contribution of at least one parameter to a plurality of experiments of the set of experiments based on the contribution of one or more other parameters to one or more of the experiments in the set of experiments.

78. The method of claim 72, wherein:

the constraints include a list constraint identifying a list of one or more starting compositions to be used to generate the set of experiments.

79. The method of claim 72, wherein:

the constraints include a synthesis constraint specifying an order in which a plurality of component materials are to be added in a synthesis to be performed in one or more of the experiments in the set of experiments.

80. The method of claim 79, wherein:

the synthesis constraint specifies that the order in which component materials are to be added is to vary between a plurality of experiments in the set of experiments.

81. The method of claim 72, wherein:

the constraints include a process constraint specifying an order in which a plurality of process steps are to be performed in one or more of the experiments in the set of experiments.

82. The method of claim 81, wherein:

the process constraint specifies that the order in which process steps are to be performed is to vary between a plurality of experiments in the set of experiments.

83. The method of claim 70, wherein:

the constraints include a project constraint specifying the order in which individual experiments in the set of experiments are to be performed.

84. The method of claim 70, wherein:

at least one of the constraints includes one or more tolerance values representing an amount by which the corresponding constraint can be relaxed during generation of the experiment design.

85. The method of claim 70, wherein:

the set of experimental parameters includes at least ten experimental parameters.

86. The method of claim 70, wherein:

the final set of experiments includes at least 1,000 experiments.

87. The method of claim 72, wherein:

each of the component materials has an associated set of material properties describing the component material; and

defining the set of experimental parameters includes specifying for each of the component materials a set of values for one or more of the material properties associated with the component material.

88. The method of claim 87, wherein:

at least one of the material properties is selected from the group consisting of molecular weight, equivalents, density and concentration.

89. The method of claim 87, wherein:

at least one of the material properties is a type describing a class of chemicals to be used in generating the experiment design.

90. A computer-implemented experiment design system, comprising:

means for defining a set of experimental parameters, one or more sampling patterns defining a sampling for each parameter of the set of experimental parameters, and one or more constraints limiting the set of experiments to a particular volume or volumes of a hyperspace defined by the set of experimental parameters, at least a plurality of the set of parameters being grouped according to a parameter type such that the grouped parameters are constrained to perform a common role in the set of experiments;

means for generating an estimate of the practicability of a set of experiments defined by the parameters, the sampling patterns and the constraints, the first estimate including a count of the set of experiments defined by the set of experimental parameters, the sets of values and the constraints;

means for generating, in response to a user input approving of the estimate, an experiment design defined by the parameters, the sampling patterns and the constraints, the experiment design including a final set of experiments.

91. The experiment design system of claim 90,wherein:

the experiment design includes data representing a plurality of sets of coordinates in the hyperspace defined by the set of experimental parameters, each of the sets of coordinates defining an experiment in the final set of experiments, the system further comprising:

means for synthesizing based on the experiment design one or more combinatorial libraries including a plurality of compositions defined by the coordinates of the experiment design.

92. The experiment design system of claim 91, wherein:

the set of experimental parameters includes at least ten experimental parameters.

93. The experiment design system of claim 91, wherein:

the final set of experiments includes at least 1,000 experiments.

94. A computer program product on a computer-readable medium for designing a set of experiments, the program comprising instructions operable to cause a programmable processor to:

define a set of experimental parameters, one or more sampling patterns defining a sampling of each parameter of the set of experimental parameters, and one or more constraints limiting the set of experiments to a particular volume or volumes of a hyperspace defined by the set of experimental parameters, at least a plurality of the set of parameters being mixture parameters defining a plurality of component materials to be used in the set of experiments to generate a mixture, the sampling patterns defined for the mixture parameters defining a non-uniform sampling of the mixture parameters; and

generate an experiment design defined by the parameters, the sampling patterns and the constraints, the experiment design including a final set of experiments.

95. The computer program product of claim 94, wherein:

the experiment design includes data representing a plurality of sets of coordinates in the hyperspace defined by the set of experimental parameters, each of the sets of coordinates defining an experiment in the final set of experiments, such that the experiment design is capable of being implemented to cause a computer-controlled combinatorial synthesis process to perform the final set of experiments.

96. A computer program product on a computer-readable medium for designing a set of experiments, the program comprising instructions operable to cause a programmable processor to:

define a set of experimental parameters, one or more sampling patterns defining a sampling of each parameter of the set of experimental parameters, and one or more constraints limiting the set of experiments to a particular volume or volumes of a hyperspace defined by the set of experimental parameters, at least a plurality of the set of parameters being mixture parameters defining a plurality of component materials to be used in the set of experiments to generate a mixture, the constraints including a mixture constraint limiting the fractional contribution of at least a plurality of the component materials to a total

composition in one or more of the experiments in the set of experiments, the mixture constraint including one or more tolerance values representing an amount by which the mixture constraint can be relaxed during generation of an experiment design; and

generate an experiment design defined by the parameters, the sampling patterns and the constraints, the experiment design including a final set of experiments.

97. The computer program product of claim 96, wherein:

the experiment design includes data representing a plurality of sets of coordinates in the hyperspace defined by the set of experimental parameters, each of the sets of coordinates defining an experiment in the final set of experiments, such that the experiment design is capable of being implemented to cause a computer-controlled combinatorial synthesis process to perform the final set of experiments.

98. A computer program product on a computer-readable medium for designing a set of experiments, the program comprising instructions operable to cause a programmable processor to:

define a set of experimental parameters, one or more sampling patterns defining a sampling of each parameter of the set of experimental parameters, and one or more constraints limiting the set of experiments to a particular volume or volumes of a hyperspace defined by the set of experimental parameters, at least a plurality of the set of parameters being mixture parameters defining a plurality of component materials to be used in the set of experiments to generate a mixture, the constraints including a balance constraint limiting the contribution of at least one of the mixture parameters to the experiment design based on the contribution of a plurality of other mixture parameters to one or more of the experiments in the set of experiments; and

generate an experiment design defined by the parameters, the sampling patterns and the constraints, the experiment design including a final set of experiments.

99. The computer program product of claim 98, wherein:

the experiment design includes data representing a plurality of sets of coordinates in the hyperspace defined by the set of experimental parameters, each of the sets of coordinates

defining an experiment in the final set of experiments, such that the experiment design is capable of being implemented to cause a computer-controlled combinatorial synthesis process to perform the final set of experiments.

100. A computer-implemented method for designing a set of experiments, comprising:

defining a set of experimental parameters, the set of experimental parameters including at least four mixture parameters, each of the mixture parameters being associated with a component material to be used in the set of experiments, each of a plurality of the set of experiments including the formation of a mixture of the component materials and the reaction of the mixture to form a product, and identifying the parameters to an experiment design system;

selecting one or more sampling patterns defining a sampling for each of the parameters and providing the sampling patterns as input to the system;

defining one or more constraints limiting experiments in the set of experiments to a particular volume or volumes of a hyperspace defined by the set of experimental parameters and providing the definition of the constraints to the system;

receiving from the system an estimate of the practicability of the set of experiments defined by the parameters, the sampling patterns and the constraints, the first estimate including a count of the set of experiments defined by the set of experimental parameters, the sets of values and the constraints;

if the estimate indicates that the set of experiments is not practicable, modifying at least one of the set of parameters, the sampling patterns or the constraints, and receiving a second estimate of the practicability of the set of experiments; and

if the estimate indicates that the set of experiments is practicable, approving of the estimate, and generating an experiment design defined by the parameters, the sampling patterns and the constraints, the experiment design defining one or more combinatorial libraries of materials including a plurality of members, each of a plurality of the members corresponding to a different experiment of the set of experiments and including a different mixture of the at least four component materials associated with the mixture parameters, the experiment design providing for the mixture of each of the component materials before the reaction of the component materials to form the product.